Large-Scale Dislocation Dynamics Simulation of Bulk Deformation

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In most engineering-level calculations of materials response, the deformation properties are described by empirical constitutive relations, usually in terms of the stress, strain, strain rate, etc. The quality of the predictions of materials behavior in such calculations depends largely on the fidelity of the constitutive relations. These relations consist of sets of models designed to describe different aspects of materials deformation, with the overall parameters found by comparing the net behavior to experiment. Thus, while it is possible to infer some information about the accuracy of the models that make up the constitutive relation, it is not possible, in general, to directly test the underlying physics of the individual models. The overall goal of this project is to develop better understanding and phenomenology of the fundamental processes of deformation and to use that to create better descriptive models for use in engineering-level simulations.

Plastic deformation in crystalline metals is a consequence of the collective motion of large numbers of dislocations, which are curvilinear defects that interact via complex, long-ranged interactions. In a typical deformable material, such as a metal, dislocation densities range from about 10^{10} to $10^{15}/m^2$, i.e., 10^{10} to 10^{15} meters of dislocations in a cubic meter of material, values that typically increase rapidly under applied stress (or strain). The mobility of dislocations gives rise to plastic flow at relatively low stress levels compared to the theoretical strength. Dislocations form organized structures such as walls, cells and pile-ups. Differences owing to the topological constraints placed by crystallography greatly add to the complexity of describing dislocation microstructural evolution and dynamics.

To develop a better understanding of the complexity of dislocation structures and dynamics, we have been developing a robust computer simulation method employing the technique of Dislocation Dynamics (DD). In DD simulations, the underlying atomic structure is ignored, the dislocations are the simulated entities and their movement is tracked during the simulation. In the past few years, there has been an increasing use of direct three-dimensional simulation of the evolving dislocation microstructures employing the DD technique. There are a number of groups working to develop these methods, including the Advanced Simulation and Computing (ASC) program at Lawrence Livermore National Laboratory and others. Dislocation Dynamics simulations are very expensive computationally, limiting the maximum stress, and the consequent dislocation density, that can be applied to the sample. They can, however, provide "data" about specific processes not available experimentally, which can then be used in the development of models of deformation.

Recently Ghoniem and his group at University of California at Los Angeles have developed a new approach to DD simulations, in which the dislocations are described as a set of nodes and a spline interpolation between the nodes is employed to determine the location of the dislocation line. The forces and energies are obtained by numerical integrations along the loops. While this approach is very promising, a great deal of computational development is needed before it could handle sufficiently large numbers of dislocations to be applied to problems of interest. Rather than develop a Los Alamos National Laboratory version of his code, we have begun a collaboration to develop a parallel 3D DD code that employs a multipolar expansion for the stress, which reduces the computational burden tremendously.

The first step in our collaboration was to ensure that the basic methodology was sound. In a collaboration with an experimental effort in the Materials Science and Technology Division (funded through

Office of Science), we performed the first detailed comparisons between discrete dislocation simulations and experiments [1]. In the experiments, the 3D position of a set of dislocations in a thin foil of copper was determined. The system was strained and then the new positions were found. We started the simulations at the experimental initial conditions, applied the same strain, and calculated the final positions. In Fig. 1 we show a comparison between the experimental and calculated final positions. The good agreement between experiment and simulations results shows that the basic methodology is sound.

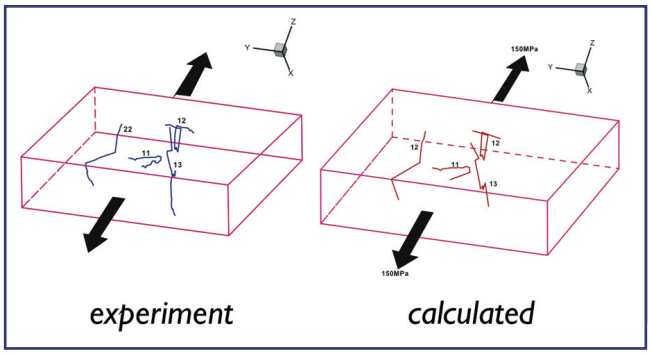

Figure 1— Experimental and calculated dislocation positions. This was the first study to directly compare calculated dislocation motion and experimental results in three dimensions.

Once we had assured ourselves as to the accuracy of the method, we began a project to improve the computations. We started by creating a parallel version of the dislocation dynamics code, based on the hierarchical tree structure developed in the MONDO project (M. Challacombe, T-12, also supported by the ASC program) [2]. We find very good scaling, with a loss of efficiency of less than 15% up to about 60 processors. In Fig. 2, we show simulated dislocation microstructures in copper at 0.1% strain. Note the beginnings of the development of structure. Parallelization is not sufficient, however, as dislocations interact with long-range forces, with a computer time that scales as the square of the length of dislocations. To achieve much higher dislocation densities, we are implementing a multipole method to reduce computational time to be approximately linear with the length of dislocations [3].

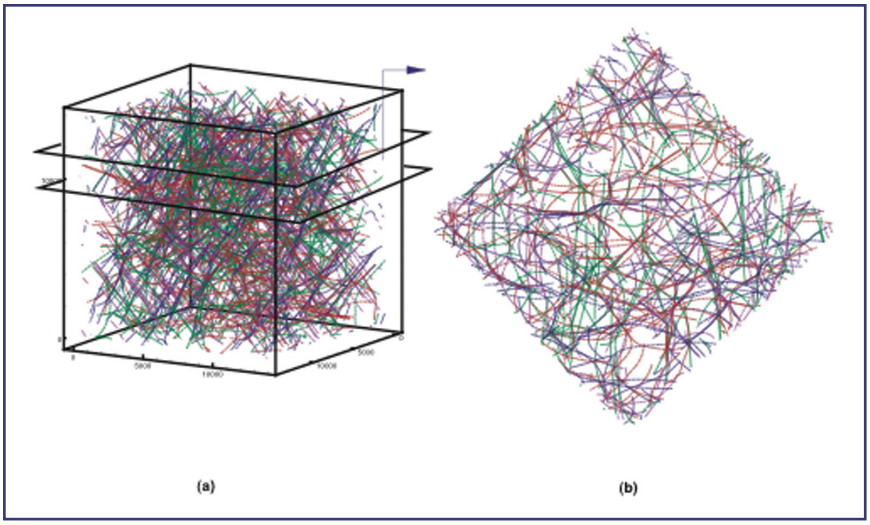

Figure 2— (a) Calculated dislocation microstructure in copper strained to 0.1%. The colors indicate the slip plane. The system size is 5 μm × 5 μm × 5 μm. (b) A view through the slice shown in the full cube. The final dislocation density is about 1.45 × 10^{13}/m^2.

We are now well poised to begin detailed simulations of the fundamental processes of deformation at a dislocation level. The next steps are to finish implementation of the multipole methods and to port the parallel code to Los Alamos machines with much larger number of processors. We will then be able to simulate dislocation structures and dynamics in real systems under conditions of interest to Los Alamos.

[1] Z. Wang, et al., "Dislocation Motion in Thin Cu Foils: A Comparison between Computer Simulations and Experiment," *Acta Mater.* **52**, 1535-42 (2004).
[2] Z. Wang, et al., "Parallel Algorithm for 3D Dislocation Dynamics," submitted to *J. Comput. Phys.*
[3] Z. Wag, N.M. Ghoniem, and R. LeSar, "Multipole Representation of the Elastic Field of Dislocation Ensembles," *Phys. Rev. B* **69**, 174102 (2004).

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